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13. ABSTRACT (Maximum 200 words)  The primary objective of this research has been to give strategies for improving shape memory and magnetostrictive materials based on reliable mathematical and computational models. Our theoretical research has led to the prediction of a new type of material, that combines the shape memory and magnetostrictive effects. Also, relying on experimental data obtained in our laboratory, we have been led to model the kinetics and hysteresis in a Cu-Al-Ni shape memory alloy by a new "wiggly energy" concept: many little wiggles are superimposed on the energy to reflect small scale microstructural changes. We have developed has rigorous theory for the analysis of the approximation of microstructure which will allow the development of efficient and reliable numerical methods for microstructure. Our research group has also developed methods and codes which have been used to compute complex equilibrium and dynamical microstructures.				
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Transitions and Defects in Crystals

December 16, 1991 – December 15, 1995

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STATEMENT OF PROBLEM STUDIED

In general, the central problem to be overcome is to find better materials. For a wide spectrum of technologies the main bottleneck is that current materials fall short of desired performance goals. While design, control and processing are all important in reaching these goals, the main issue is the materials themselves. The specific goal of this research is to give strategies for improving shape memory and magnetostrictive materials based on reliable mathematical models, studied via modern computational methods. The improvements are aimed at actuator applications.

The main opportunity to be seized at this time in the study of materials is the behavior and synthesis of materials at small scales. The emerging near-term route is thin films. It is becoming possible to synthesize many small scale devices on a wafer using integrated circuit technology. The field is now entirely driven by experiment; new methods are tried that are experimental extensions of what worked previously. Mathematical modeling and computation have an important role to play in this area, by predicting beforehand what properties are expected and by providing optimal designs. There is real chance for new discoveries here, as thin films behave entirely differently from bulk materials.

Our theoretical research has led to the prediction of a new type of material, that combines the shape memory and magnetostrictive effects. We have termed such a material a "magneto-memory" material. We have given a strategy for finding such a material, based on 1) arranging a martensitic transformation to be near a ferromagnetic transition, and 2) adjusting the lattice parameters of the material to satisfy "special relations" that promote desirable domain structures for microstructural rearrangements. This new material is predicted to have magneto-elastic strains that are more than

an order of magnitude larger than current giant magnetostrictive materials. This strategy is now being implemented by Wuttig and James.

There are two main puzzles in the mathematical modeling of active materials, that directly affect actuator applications. They are the related topics of hysteresis and kinetics. A new model of the kinetics of transformation between two variants of martensite has been given, based on a "wiggly energy" concept (see below). This shows good agreement with experiment, for a wide variety of different experiments: inner and outer hysteresis loops, creep tests, and various far from equilibrium tests. More importantly, it gives an understanding of the origins of hysteresis in terms of microstructure.

The main potential payoff is new materials for ARO applications. We aim for very specific strategies to be used for the improvement of materials, and explicit mathematical models. We do not do phenomenological modeling; the models we develop are based on fundamental transformation properties, such as lattice parameters, crystallographic symmetries, latent heat, saturation magnetization, etc. The reason for this approach is that the mathematical and computational models can then be used in the direct design of materials, by asking the question (as we do) of how do the predictions change when the fundamental properties change. More importantly, we look for special properties that give unusual or optimal behavior.

Since this research gives such explicit predictions, it entails a certain amount of risk. The predictions are periodically checked by direct comparison with experiment (currently by Tickle, Wuttig, De Graef).

## SUMMARY OF MOST IMPORTANT RESULTS

Our theoretical research has led to the prediction of a new type of material, that combines the shape memory and magnetostrictive effects. We have termed such a material a "magneto-memory" material. We have given a strategy for finding such a material, based on 1) arranging a martensitic transformation to be near a ferromagnetic transition, and 2) adjusting the lattice parameters of the material to satisfy "special relations" that promote desirable domain structures for microstructural rearrangements. This new material is predicted to have magneto-elastic strains that are more than an order of magnitude larger than current giant magnetostrictive materials. This strategy is now being implemented by Wuttig and James. The existence of

such a material became clear after studies of giant magnetostriction [18]

There are two main puzzles in the mathematical modeling of active materials, that directly affect actuator applications. They are the related topics of hysteresis and kinetics. Relying on the experiments of Chu [10], Abeyaratne, Chu and James [2, 1] have been led to model the kinetics and hysteresis in a Cu-Al-Ni shape memory alloy by a new “wiggly energy” concept: many little wiggles are superimposed on the energy to reflect small scale microstructural changes. In this alloy the wiggles are due to the presence of thousands of tiny needles in the specimen [20], and the passage out of a local minimum corresponds to a tip splitting event. The predictions show good agreement with experiment, for a wide variety of different experiments: inner and outer hysteresis loops, creep tests, and various far from equilibrium tests. More importantly, the model gives an understanding of the origins of hysteresis in terms of microstructure. The idea has been extended to the analysis of the friction between clean surfaces [24], giving a model that explicitly relates the surface roughness to static friction (The authors are currently trying to predict roughness profiles that minimize or maximize friction; they also have set up a simple experimental program to measure the surface roughness of various surfaces by the atomic force microscope and then to compare the predictions of theory with measurements of macroscopic static friction).

Together with G. Gioia [13] and K. Bhattacharya [9], James has recently been trying some thin film calculations. By scaling a film thinner and thinner, it is found there is a mismatch of terms of the energy: certain terms are much larger than others. This can be used as the basis of a rigorous asymptotic argument giving a general limiting thin film theory. We have tried out this kind of argument for micromagnetic and martensitic energies. The results look to be extremely useful for predicting the behavior of this films, and point to major advantages of epitaxy.

Luskin gave the first analysis of the approximation of martensitic microstructure for a physically realistic, multi-dimensional crystalline energy [30, 31]. He developed this analysis for the orthorhombic to monoclinic (double well) transformation [31] and then extended the analysis with his graduate student, Bo Li, to the cubic to tetragonal (triple well) transformation [29]. He applied the approximation theory developed in his analysis of microstructure to obtain error estimates for the numerical approximation of microstructure by the finite element method. This analysis gives a theoretical basis for the computational projects described in the proposal and should make possible the development of more effective and reliable algorithms.

Luskin and his post-doc, Peter Klouček, have developed methods and a code to investigate fully three-dimensional dynamical phenomena associated with the propagation of the interface separating the martensitic and the austenitic phase in some indium-thallium shape-memory alloys [27, 28]. This dynamical problem is extremely challenging since the multi-well structure of the energy density leads to an ill-posed problem (in the absence of surface stress and viscous stress) for the linearized momentum equation about some strains. They have been able to develop stable time-discretization methods and efficient techniques for the solution of the linear equations at each time step even though the energy density is non-convex.

The computational experiments of Luskin and Klouček have simulated the development of martensitic microstructure and the propagation of the austenitic-martensitic phase boundary which separates the homogeneous austenitic phase from the microstructured martensitic phase. They have also done computational studies of the effects of surface stress and viscous stress on the dynamics. In [26], Klouček, Li, and Luskin have given an analysis of a nonconforming finite element method which has been used successfully to compute the dynamics of the martensitic transformation [27].

Luskin and his graduate student Bo Li have developed a numerical model for the simulation of the biaxial experiments of Chu described in [10, 5, 11].

In some shape memory alloys certain atomic scale relaxation effects take place that significantly affect long term performance. It is particularly prevalent in the Cu-based materials, and in several cases makes unusable otherwise good shape memory alloys. A new nonlinear dynamic model of this relaxation was given [8]. It shows excellent agreement with experimental measurements of the slow evolution of hysteresis loops, and the long-time "creep" of transformation temperature.

New methods for analyzing microstructure have been given, following our earlier work [3, 7].

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